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RADIATION RESEARCH ASSOCIATES, INC.

Fort Worth, Texas

COHORT

**A MONTE CARLO PROGRAM FOR CALCULATION
OF RADIATION HEATING AND TRANSPORT**

**Volume I: Modification and Verification
of Improved Version of COHORT**

D. G. COLLINS and M. B. WELLS

Prepared Under Contract NAS8-20195 for
**THE GEORGE C. MARSHALL SPACE FLIGHT CENTER,
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION,
Huntsville, Alabama**

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ABSTRACT

The family of routines designated as COHORT was recoded in FORTRAN-IV language and several improvements were made in the routines in order to increase their efficiency and to widen their range of application to radiation heating and transport problems. Every effort was made to discover and correct all coding errors in the updated version of COHORT and the accuracy of the calculational methods used in the code was checked out through comparisons of results from test problems with data from other calculational methods.

A discussion of the modifications made to COHORT and comparison of results from the FORTRAN-IV version of the code with data from other calculational methods are given in Volume I of this report. Utilization instructions for the FORTRAN-IV version of the primary source generator routine, S01, the secondary source generator routine, S02, and the tape read routine, C01, are contained in Volume II. Utilization instructions for the history generator routine, H01, and the tape sort routine, J01, are contained in Volume III. Utilization instructions for the two analysis routines, A01 and A02, are contained in Volume IV.

FOREWORD

The authors wish to acknowledge the work of all those who have participated in the development of the COHORT code, especially D. M. Braddock, L. M. Bostick, C. F. Malone and T. W. DeVries who shared in the coding of the original version of COHORT. They wish to express their appreciation to Mr. Len Soffer and Mr. Irv Karp for their work in translating COHORT to FORTRAN-IV and for their suggestions for improvements to the code. They also wish to express their appreciation to Mr. James Price and Mrs. Linda Causey for their help in debugging the current version of COHORT. The authors are appreciative of the guidance provided by Mr. Henry Stern, the technical monitor of both the previous and current studies for the development and improvement of COHORT.

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I INTRODUCTION

COHORT (Ref. 1 & 2) is a generalized geometry Monte Carlo program designed to calculate the radiation environment and nuclear energy deposition within a complex geometry system such as a nuclear rocket stage. The flexibility offered in geometry description and the analysis routines provided in the COHORT program facilitates the application of the program to a wide range of shielding and radiation transport problems.

The set of seven codes comprising the COHORT program was developed and coded in FORTRAN-II at the Nuclear Aerospace Research Facility operated by General Dynamics/Fort Worth. The program was converted to FORTRAN-IV by personnel at NASA Lewis Research Center and their attempted use of the program indicated the need for further checkout.

The purpose of the work reported in this document was to complete the checkout of the FORTRAN-IV version of the COHORT program and to improve the method used to input cross section data. Several other minor changes were made in the coding to increase the efficiency of the program. A detailed discussion of the improvements made in the COHORT program is given in Section II.

Several problems were run to check the validity of the improved version of the COHORT program and a discussion of these problems is given in Section III.

Some of the improvements made in the COHORT program required that changes be made in the input data formats. The utilization instructions for the seven codes have been rewritten and are included in Volumes II, III and IV of this report.

II MODIFICATIONS TO COHORT

The more significant modifications made to the COHORT program are discussed below.

2.1 Cross Section Description

Modifications made to COHORT include the removal of the requirement that cross sectional data be input at equally spaced energy points within a given energy super-group. In COHORT the energy interval for a given problem may be divided into several intervals, each of which is designated as an energy super-group. The total, scattering and elastic cross sections for neutrons or the total, Compton plus pair production, and Compton cross sections for gamma rays can now be input for up to 100 arbitrarily spaced energy points within any super-group. The requirement still remains in the program that for a given super-group, the set of energy points used in defining the cross sections must be the same for all elements. The energy points at which cross sections are input are read into memory each time that the cross sections for a given element are read-in. The energy points read-in for each succeeding element are stored in the same memory locations used for the previous element so that energy points for the cross sections read-in for the last element are used as the energy points for all elements. Cross sections for any given energy are calculated by locating the two input energy points that bound the energy of interest, and interpolating linearly between those two energies to obtain the cross section for the energy of interest. A searching scheme was developed and included in the program to locate the two energy points in a given super-group that bound the working energy. Rather than comparing the working energy with

each energy point within the super-group until an energy lower than the working energy is found, the scheme involves successive divisions of the set of energy points into groups of halves, fourths, eighths, etc. then locating the half, fourth, eighth, etc. which contain the working energy. The two energy points bounding the working energy may be determined with a maximum of seven searches using the above scheme. If a point-to-point search scheme had been used, the number of searches required to locate the two energies bounding the working energy would be approximately equal to half of the number of energy points within a super-group.

2.2 Geometry Modification

Additional modifications to COHORT resulted in the generalization of the geometry to include surfaces of revolution about a line parallel to the Z axis and planes of arbitrary orientation. The program previously allowed only surfaces of rotation about the Z axis and planes normal to one of the axes or normal to the XY plane. These two changes in the COHORT geometry require the input of two additional parameters for each boundary in the boundary description table.

The equations for defining spherical, hyperbolic, elliptical, parabolic, conical and cylindrical surfaces are given below:

$$(1) \quad (X-XF)^2 + (Y-YF)^2 - AF(Z-ZF)^2 - CF = 0,$$

$$(2) \quad (X-XF)^2 + (Y-YF)^2 - AF(Z-ZF) = 0,$$

$$(3) \quad \sqrt{(X-XF)^2 + (Y-YF)^2} - AF(Z-ZF) = 0, \text{ and}$$

$$(4) \quad \sqrt{(X-XF)^2 + (Y-YF)^2} - AF = 0.$$

AF, ZF, CF, XF and YF are input parameters which are defined in Volume II.

The first equation may be used to describe spherical, hyperbolic or elliptical surfaces, the second a parabolic surface, the third a conical surface and the fourth a cylindrical surface. The equation for an arbitrarily oriented plane surface is defined by the equation, $AF \cdot X + YF \cdot Y + CF \cdot Z - YF = 0$ where AF, ZF, CF and XF are input parameters.

2.3 Correction of A02 Analysis Routine

During the checkout of the A02 analysis routine it was discovered that the flux in a region between the last collision point and an outside boundary was being underestimated. This underestimate in the flux resulted from the fact that the collision data had been recorded on the history tape for the last collision before escape and that no means were available for determining the path length from this collision to the outside boundary. This error was corrected by a modification to the H01 routine so that the point of escape would be written on the history tape as a pseudo-collision. The weight assigned to the particle after collision for pseudo-collisions was zero. The A02 code now computes the track length between the last collision point before escape and the escape point which is the pseudo-collision point.

The A01 and S02 routines were modified so that they now disregard collision data on the history tape for those collisions with zero weights after collision.

Several other minor modifications were made in the COHORT program to improve the efficiency of the program. The variables listed in the COMMON and DIMENSION statements were rearranged to make more efficient use of core storage locations and to make several of the subroutines in the H01, A01 and A02 codes interchangeable.

III VALIDATION OF COHORT PROGRAM

To establish the validity and to demonstrate the versatility of the COHORT program, several comparisons have been made between COHORT data and that generated by other methods. The calculations performed and the results obtained are presented in the following discussions.

3.1 Energy Deposition in Liquid Hydrogen

An H01 problem was run to calculate the heat deposited in a liquid hydrogen slab due to a 7 Mev plane parallel neutron source incident normal to the slab. In Figure 1 the results of the 4200 history H01 problem are compared with Burrell's data for the same problem (Ref. 3). The curve in Figure 1 represents a smooth curve drawn through Burrell's data. The circled points in Figure 1 were obtained by dividing the H01 energy deposition per region by the region thicknesses to give the energy deposition in units of $\text{Mev/cm}^{-3}\text{-sec}^{-1}$ and these data were then converted to $\text{BTU/in}^{-3}\text{-sec}^{-1}$. The good agreement between the two sets of data indicates the accuracy of the COHORT program in calculating neutron energy deposition at large depths in liquid hydrogen.

A second comparison between COHORT data and Burrell's calculations of neutron energy depositions in liquid hydrogen was made to test the application of the exponential transformation available in COHORT. In this case the energy deposited by 2 Mev neutrons incident normal to a liquid hydrogen slab was calculated in three separate COHORT problems. In the first problem no exponential transformation was applied. In the second the pseudo cross section is given by the expression

$$\bar{\Sigma} = (1 - .5\gamma)$$

where $\bar{\Sigma}$ is the pseudo cross section used in selecting path lengths, Σ is the true cross section, and γ is the directional cosine measured from

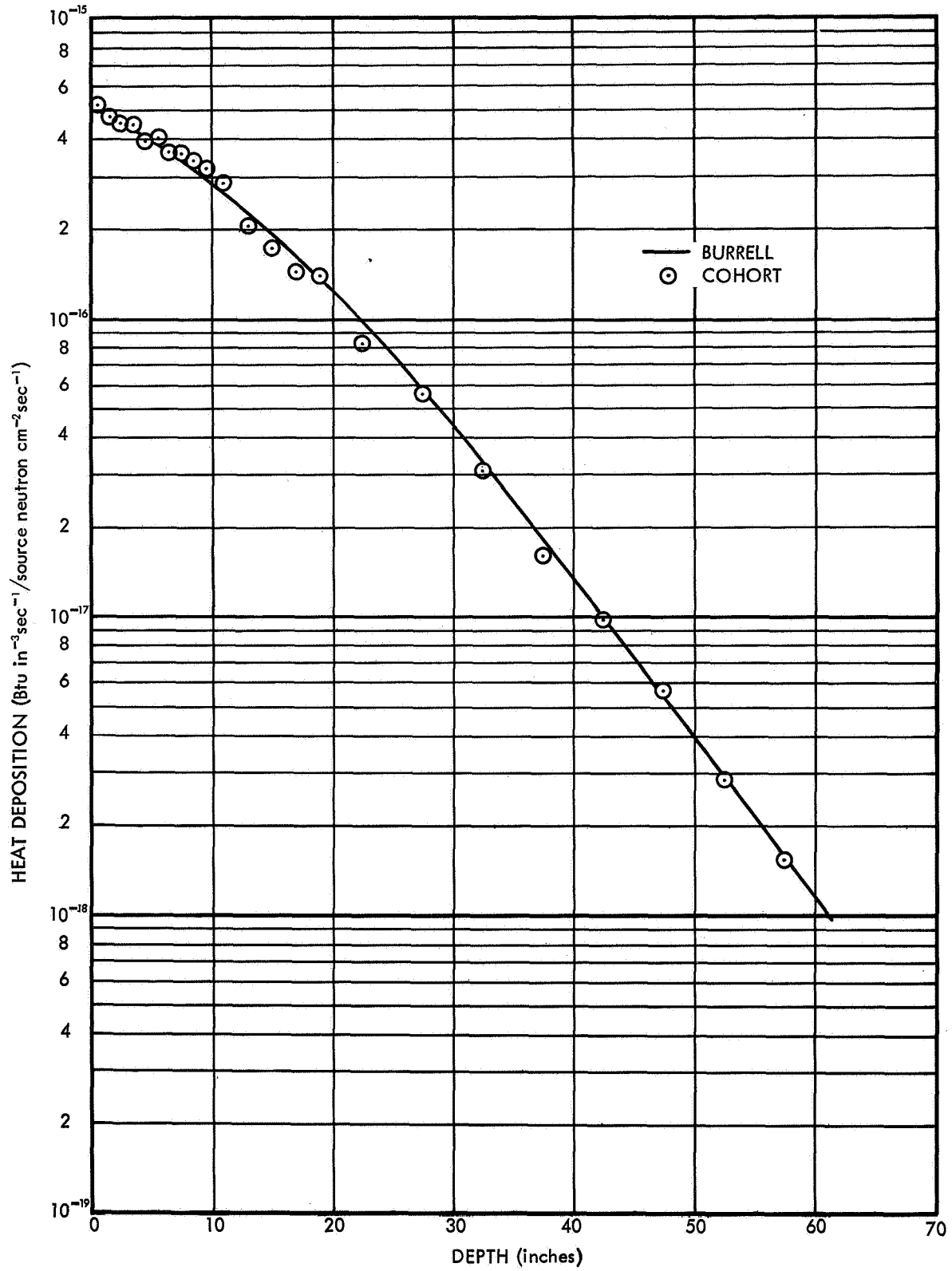


Fig. 1. Heat Deposition vs Depth in Liquid Hydrogen Slab due to 7.0 MeV Normal Incident Plane Source

the normal into the slab. When γ is negative, $\bar{\Sigma}$ is set equal to Σ . In the third problem the pseudo cross section used in the selection of path lengths is given by the expression

$$\bar{\Sigma} = \Sigma(1 - .9\gamma) .$$

Results of the three COHORT problems are compared with a smooth curve drawn through Burrell's data in Figures 2, 3 and 4. Burrell's report gives his results only to a depth of 33 inches, therefore, his data were extrapolated to 60 inches to compare with the COHORT data. The exponential transformation affected the results as anticipated. When no exponential transformation was applied, Figure 2, all histories were terminated before reaching a depth of 35 inches. By applying the exponential transformation, sampling at the larger depths was improved, Figures 3 and 4. The greater stretching of path lengths, Figure 4, did not produce a significant improvement over the results shown in Figure 3, however. The results shown in Figures 2, 3 and 4 support the conclusion reached by Jones (Ref. 4) in his investigation of the exponential transformation as used in the FMC and SPARC codes where he found that the Monte Carlo calculated quantities were insensitive to the value of b in the equation $\bar{\Sigma}_r = \Sigma_T(1 - b\gamma)$ for values of b greater than some minimum value. It is evident from the results shown in Figures 3 and 4 that further improvement in the results at depths between 30 and 60 inches will not be obtained by using a value of $b > 0.5$.

3.2 Thermal-Neutron Absorption in Concrete

A series of COHORT problems were run to calculate the absorption of thermal neutrons in a concrete slab due to a normally incident thermal-neutron plane parallel source. For these problems scattering was assumed

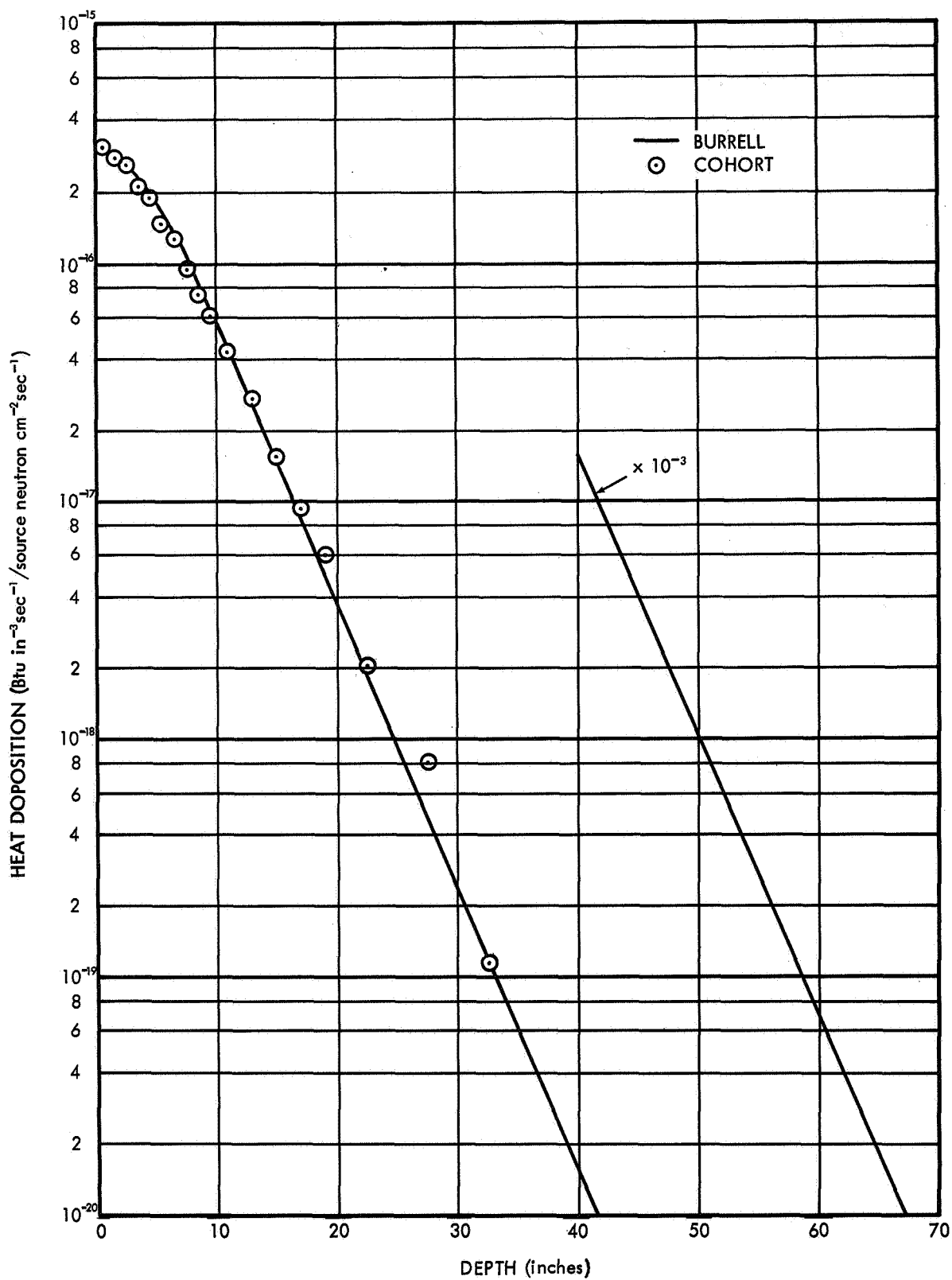


Fig. 2. Heat Deposition vs Depth in Liquid Hydrogen Slab due to 2.0 MeV Normal Incident Neutron Plane Source (no exponential transformation)

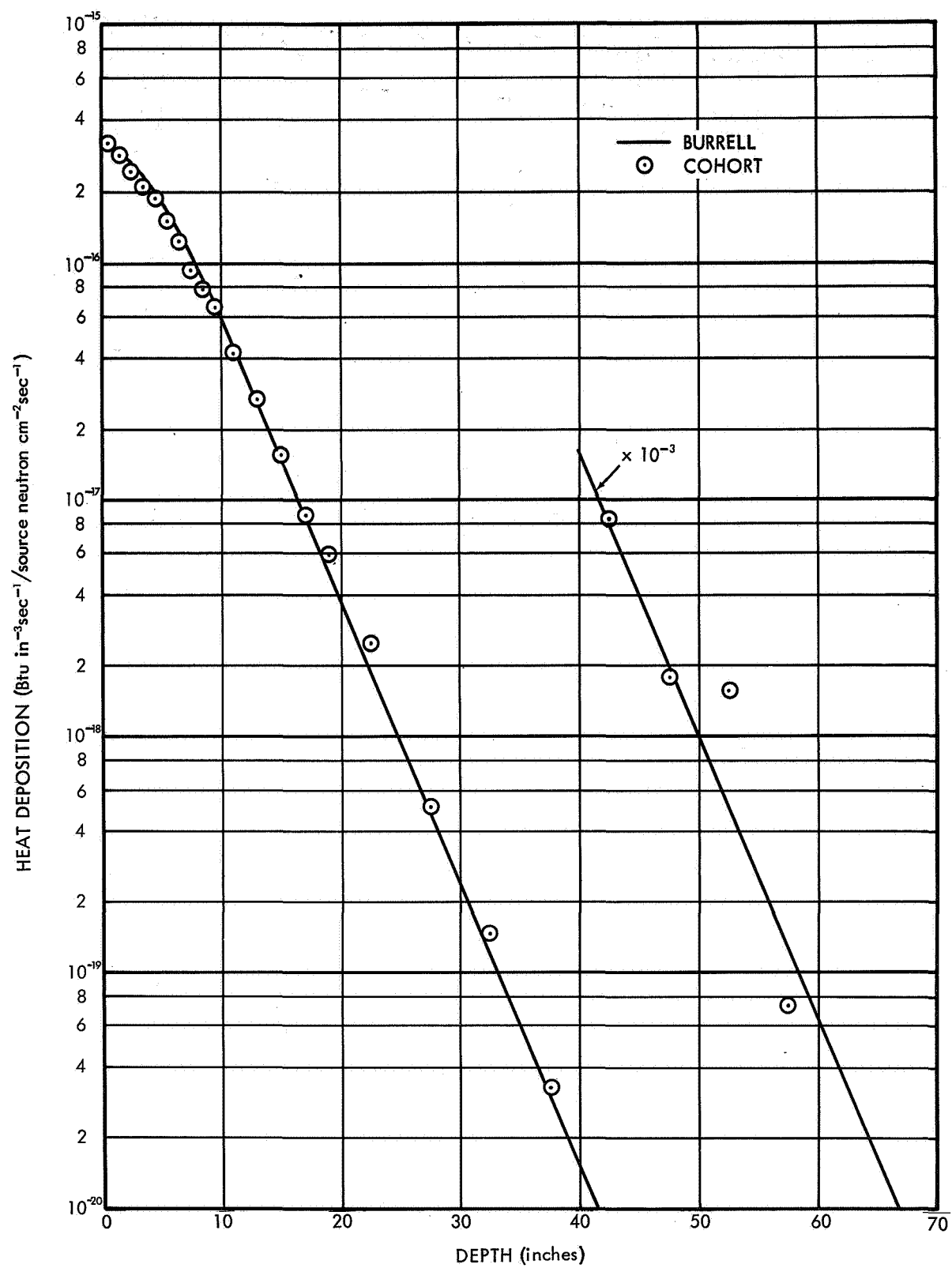


Fig. 3. Heat Deposition vs Depth in Liquid Hydrogen Slab due to 2.0 MeV Normal Incident Neutron Plane Source ($\bar{\Sigma} \approx \Sigma(1 - .5\gamma)$)

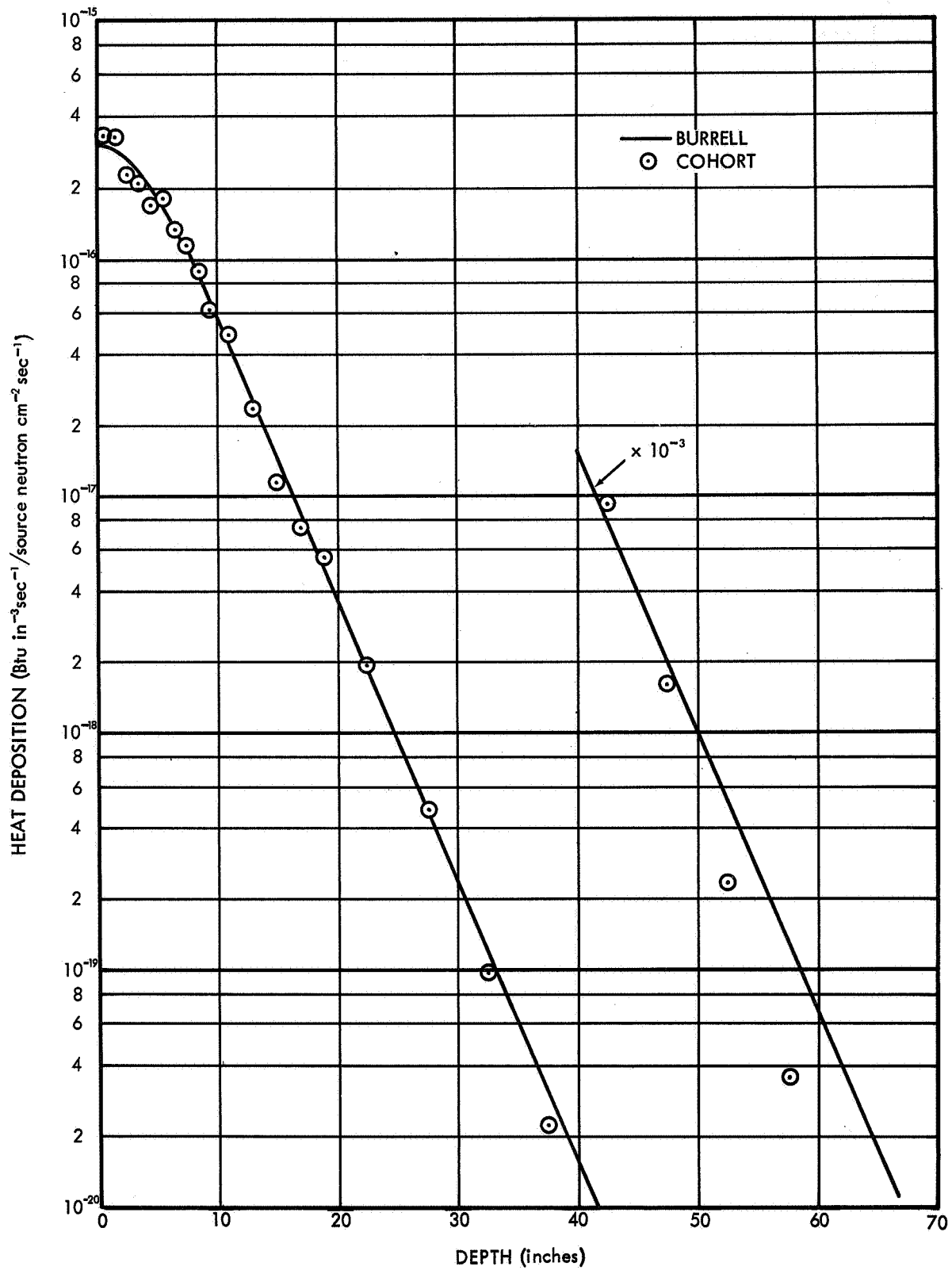


Fig. 4. Heat Deposition vs Depth in Liquid Hydrogen Slab due to 2.0 MeV Normal Incident Neutron Plane Source ($\bar{\Sigma} = \Sigma(1 - .97)$)

to be isotropic in the laboratory system with no energy degradation. The absorption-to-total cross section ratio was .013. An H01 problem was run, allowing a maximum of one hundred collisions per history, to calculate the energy deposition as a function of depth in a 66.4 cm thick concrete slab. The number of neutrons absorbed per cm^3 at a given depth in the slab was computed by dividing the energy deposited per cm^3 as the result of absorption at that depth by the energy of the neutron. The results of the H01 calculations are compared in Figure 5 with those obtained from a DTF one-energy group, S_{16} calculation, reported by Maerker and Muckenthaler (Ref. 5). The comparison with the DTF results is good to about 15 mean-free-path lengths. At the larger depths COHORT tends to underpredict the DTF results. The H01 results in Figure 5 were calculated without any application of the exponential transformation.

3.3 Thermal-Neutron Albedo for Concrete

Maerker and Muckenthaler have also reported Monte Carlo calculations of the differential thermal-neutron albedo for concrete slabs. The A02 analysis routine of COHORT was run to obtain the thermal-neutron current reflected from a 66.4 cm thick concrete slab for comparison with their values. The A02 calculated thermal-neutron current reflected from the slab as a function of the angle measured from a normal to the slab was converted to neutrons per steradian and the results are presented in Figure 6 where they are compared with the thermal-neutron albedo as calculated by Maerker and Muckenthaler.

The average number of track lengths per region in the concrete slab was obtained from the A02 analysis routine. These data were converted

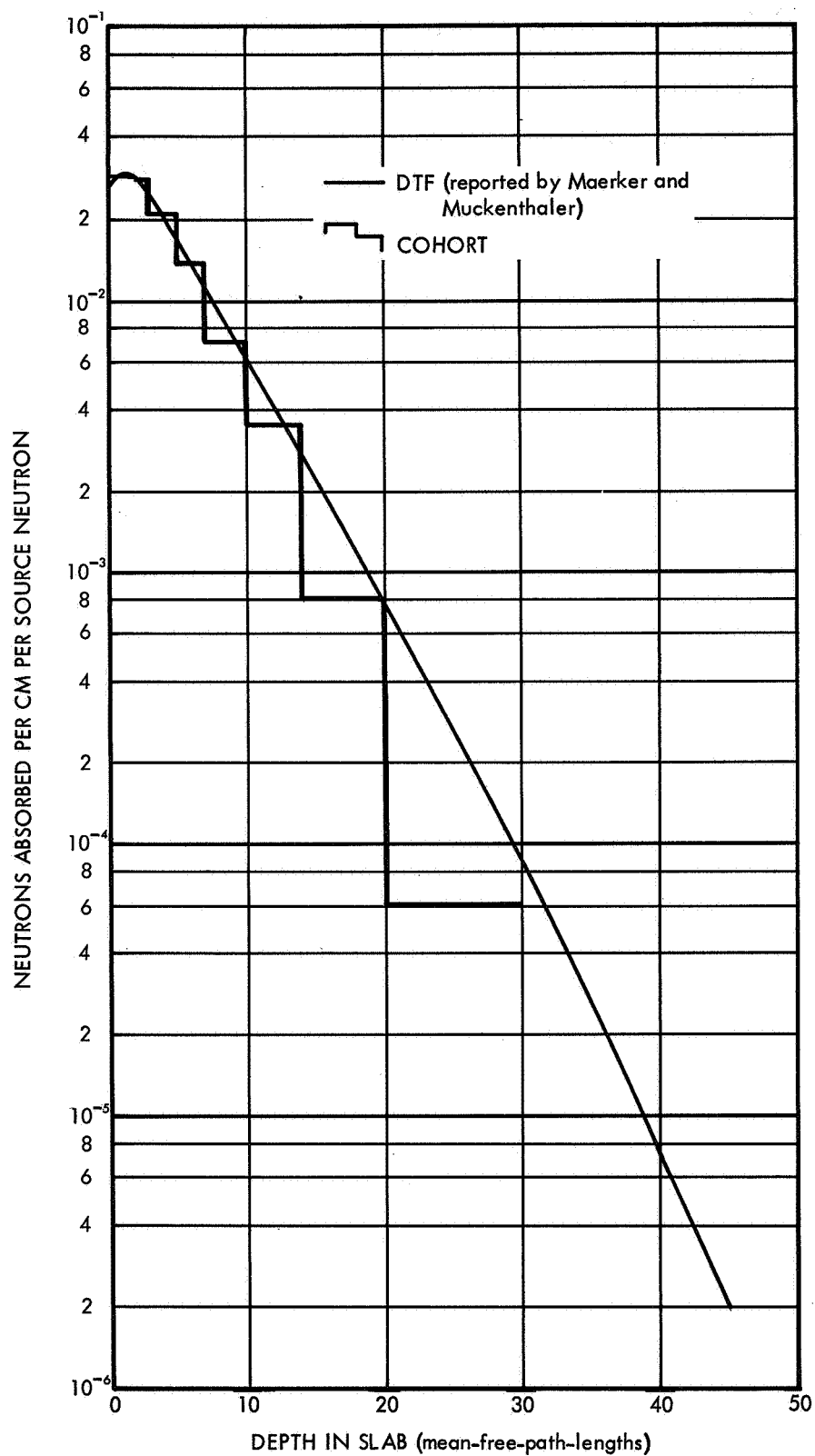


Fig. 5. Thermal Neutron Absorption as a Function of Depth in a Concrete Slab due to a Normal Incident Plane Parallel Source of Thermal Neutrons

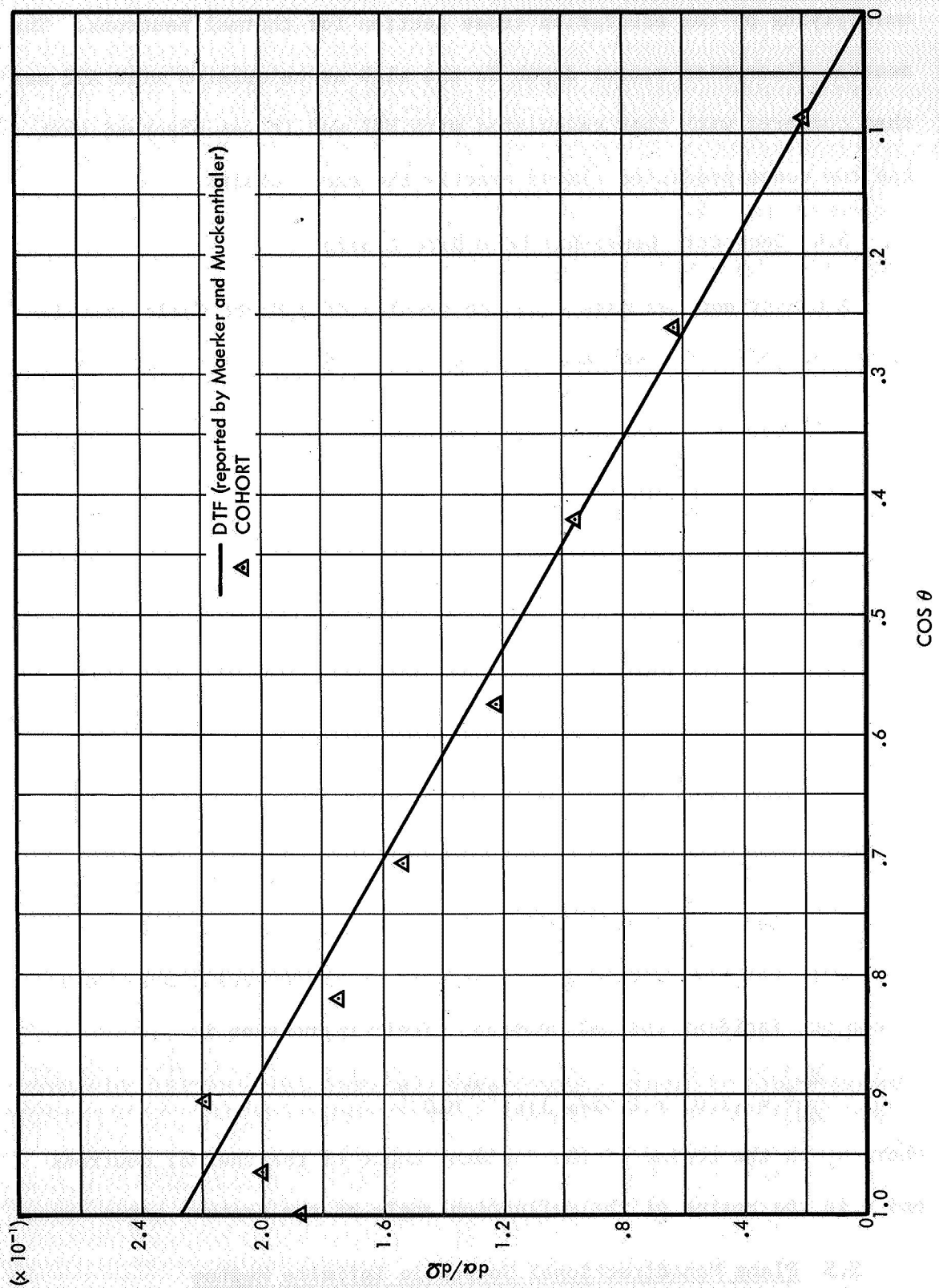


Fig. 6. Thermal Neutron Albedo for Concrete ($\Sigma_s / \Sigma_t = 0.978$)

to neutron absorption by dividing by the thickness of the region and multiplying by the absorption cross section for thermal neutrons. The neutron absorption versus depth in the slab as calculated with A02 was then compared with that calculated with H01 and it was observed that the two codes predicted almost exactly the same results.

3.4 Secondary Gamma-Ray Dose Rate Albedo

A comparison was made with the results of a Monte Carlo calculation reported by Maerker and Muckenthaler to determine the neutron capture gamma-ray dose albedo for a 66.4 cm thick concrete slab. The S02 routine was run to analyze the history tape from the H01 thermal-neutron problem and to produce a capture gamma-ray source tape. A set of capture gamma-ray histories were generated with H01 using the source tape from the S02 routine. Finally the history tape from the H01 problem generating the secondary gamma-ray histories was analyzed with the A02 analysis routine to produce the capture gamma-ray current reflected from the slab as a function of energy and angle. The A02 calculated capture gamma-ray current was converted to dose rate per steradian and the results are compared in Figure 7 with the angular distribution of the dose albedo as given by Maerker's and Muckenthaler's analytical expression for the capture gamma-ray current differential dose rate albedo per incident thermal neutron. Their expression is

$$\frac{dD}{d\Omega} = (1.03 + 1.05\sqrt{\mu_0}) |\mu|^{2/3} * 10^{-7}$$

where μ_0 is the cosine of the incident angle of the thermal neutrons and μ is the cosine of the reflection angle of the capture gamma rays.

3.5 Plane Monodirectional Source in Infinite Medium

A problem designed to calculate the radiation intensity as a function of distance on either side of a plane monodirectional monoenergetic

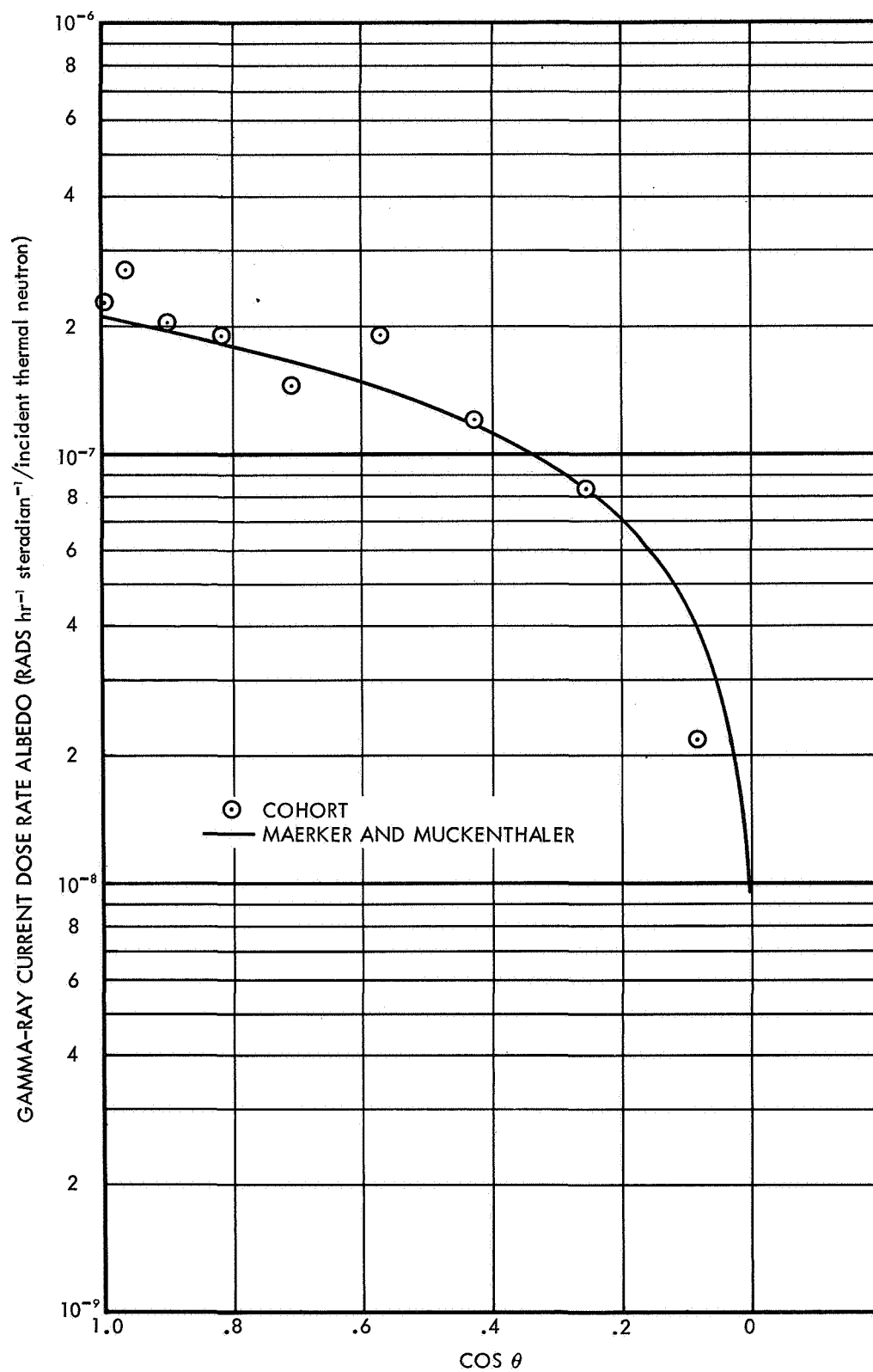


Fig. 7. Capture Gamma-Ray Current Differential Dose Rate Albedo

source in an infinite medium was run using COHORT. Scattering in the infinite medium was assumed to be isotropic with no energy degradation. The scattering-to-total cross section ratio was taken to be 0.5. Figures 8 and 9 show a comparison of the COHORT results with those reported by Beach et al. (Ref. 6) for the one velocity neutron diffusion problem. The results reported by Beach et al. were calculated using Fourier transform techniques to obtain "exact" solutions of the one-velocity neutron diffusion problem for both plane parallel and plain isotropic sources. Figure 8 shows comparisons of the total intensity on the forward side of the source plane and Figure 9 shows comparisons of the intensities behind the source plane. For the COHORT problem the infinite geometry was divided into a series of alternating thin and thick semi-infinite slab regions parallel to and on either side of the source plane. The H01 code was used to calculate the energy deposition in each of these regions and the energy deposition was converted to neutron intensity by dividing the energy deposited by the thickness of the region and the energy of the monoenergetic source. The COHORT results for the thin regions which were 0.1 of a mean-free-path length thick are indicated by the circular points in Figures 8 and 9. The COHORT results for the thicker regions are given in the form of histograms. The statistical fluctuations for the thicker regions are less than those obtained for the thinner regions, and therefore, the histograms compare more favorably with Beach's data at the larger distances.

3.6 Point Isotropic Fission Neutron Source in Air

A COHORT problem was run to calculate the neutron flux as a function of distance from a point isotropic fission neutron source in an infinite medium of air. The results of the problem are compared in

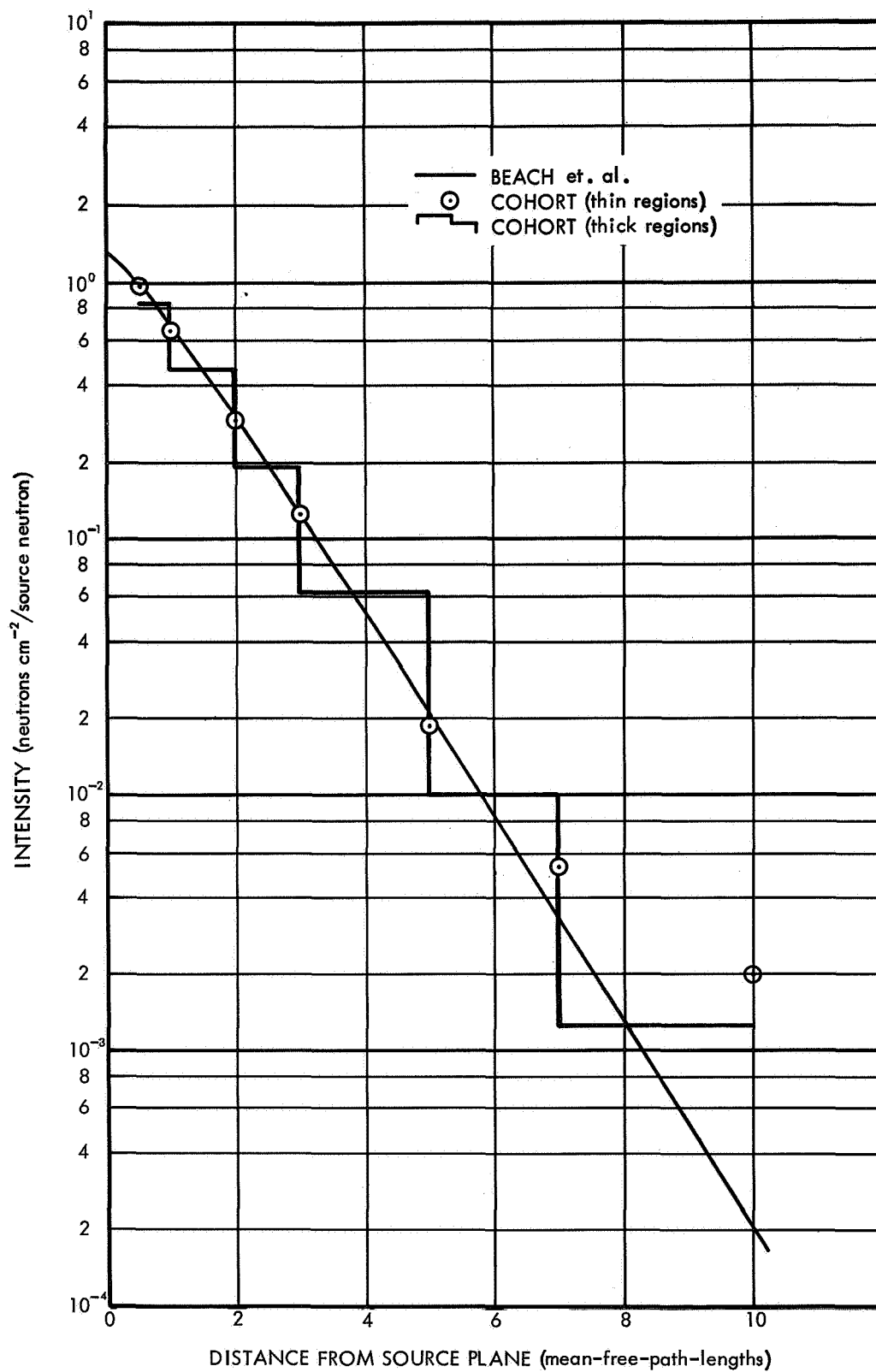


Fig. 8. Total Intensity as a Function of Distance from a Plane Monodirectional Source in an Infinite Medium ($\Sigma_s/\Sigma_T=0.5$)

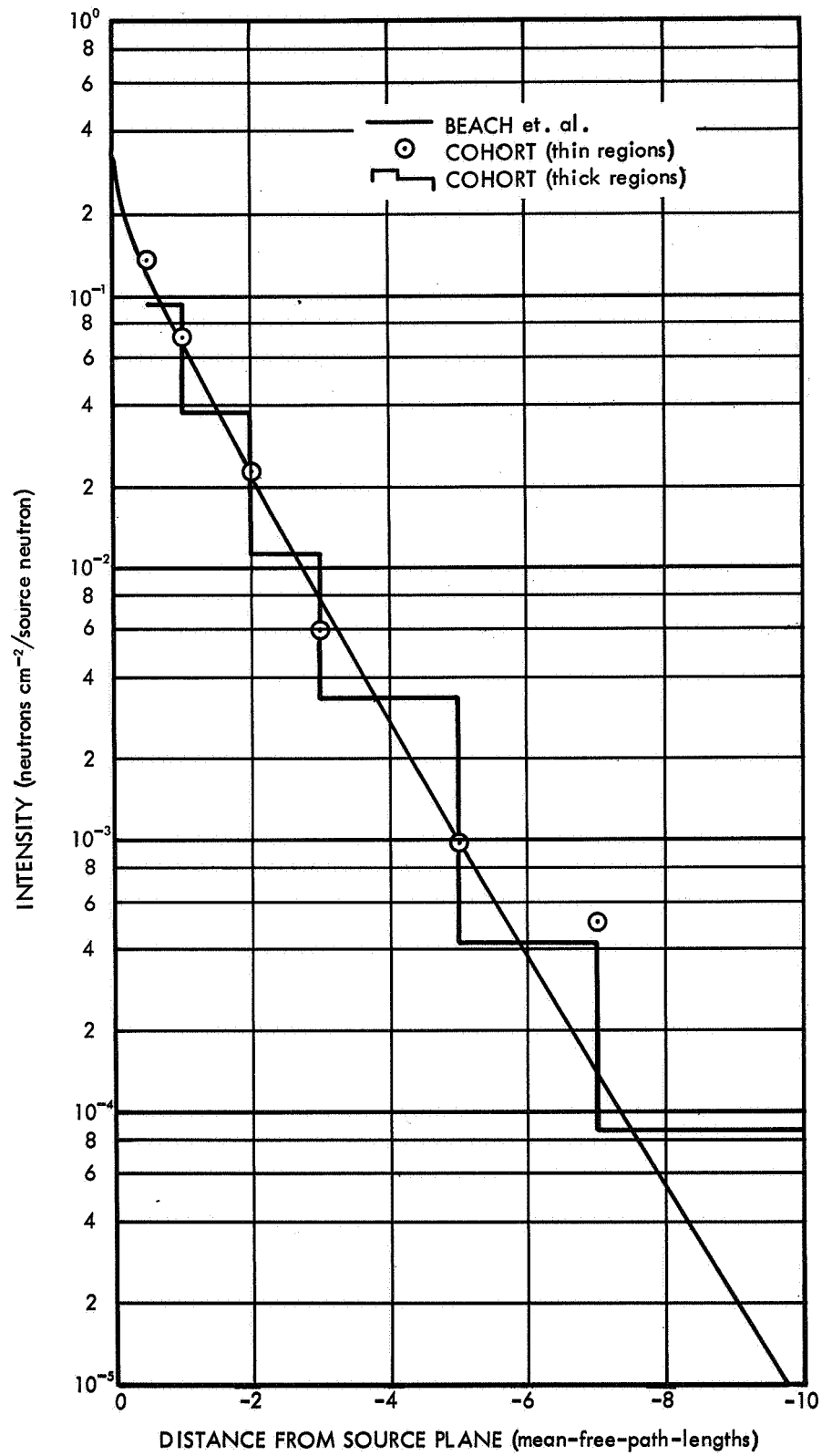


Fig. 9. Scattered Intensity Behind a Plane Monodirectional Source in an Infinite Medium ($\Sigma_s/\Sigma_T=0.5$)

Figure 10 with the results obtained when the same problem was run using the K-74 Monte Carlo code (Ref. 7). The fluxes obtained from both calculations were multiplied by $4\pi r^2$, where r is the source receiver separation distance. In the COHORT calculation the H01 and A02 routines were used to calculate the track lengths in spherical shell volumes located at radial distances of 100, 300, 750, 1200, 1500 meters from the source point. Track lengths per region were then converted to $4\pi r^2$ times the flux by dividing by the thickness of the spherical shell region. The agreement between the two calculations is reasonably good except for the point at 100 meters where COHORT overpredicts the K-74 results by about 40 percent.

3.7 Two Mev Point Isotropic Gamma-Ray Source In Air

A COHORT problem was run to provide results for comparison with K-74 data for a 2 Mev point isotropic gamma-ray source in an infinite medium of air. The comparison of the data obtained from the two different calculations are shown in Figures 11, 12 and 13. The K-74 results are for 5000 histories. Some difficulties were experienced in reading the H01 history tape when running the A02 analysis routine and only 525 histories were analyzed in the COHORT output. The agreement between the K-74 and COHORT results is very good considering the small number of histories analyzed with the COHORT code. Figure 11 shows a comparison of $4\pi r^2$ times the total gamma-ray fluxes at five receiver positions located at distances equivalent to 180, 700, 1000, 1200 and 1500 yards from the source point. The results of the two calculations are within approximately 10 percent of each other except at the 1500-yard position where COHORT overpredicts K-74 by a factor of 2.7. Figures 12 and 13 show a comparison of the energy fluxes at each of the five receiver positions.

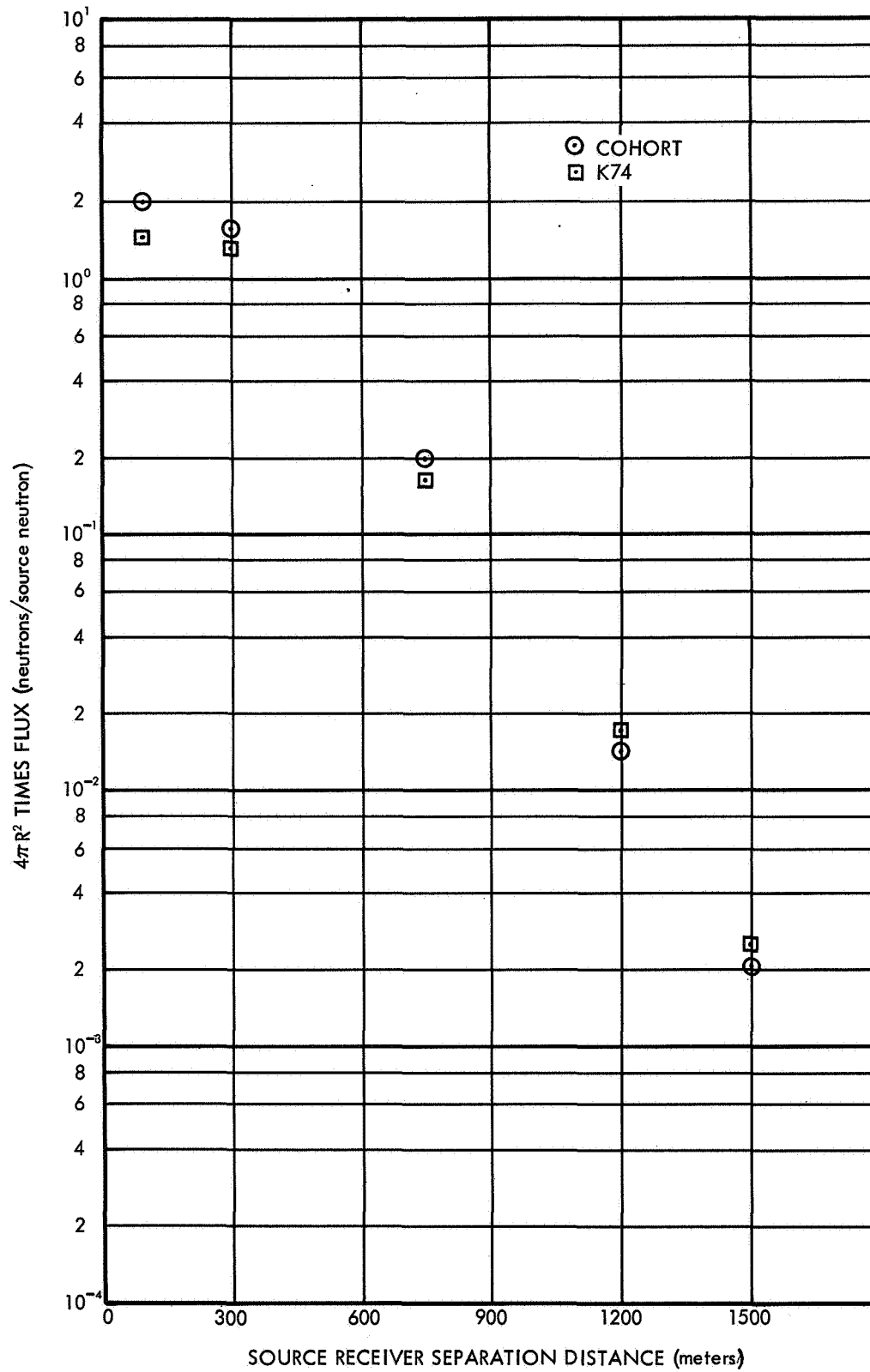


Fig. 10. $4\pi R^2$ Times Flux vs Distance from a Point Isotropic Fission Source in an Infinite Medium of Air

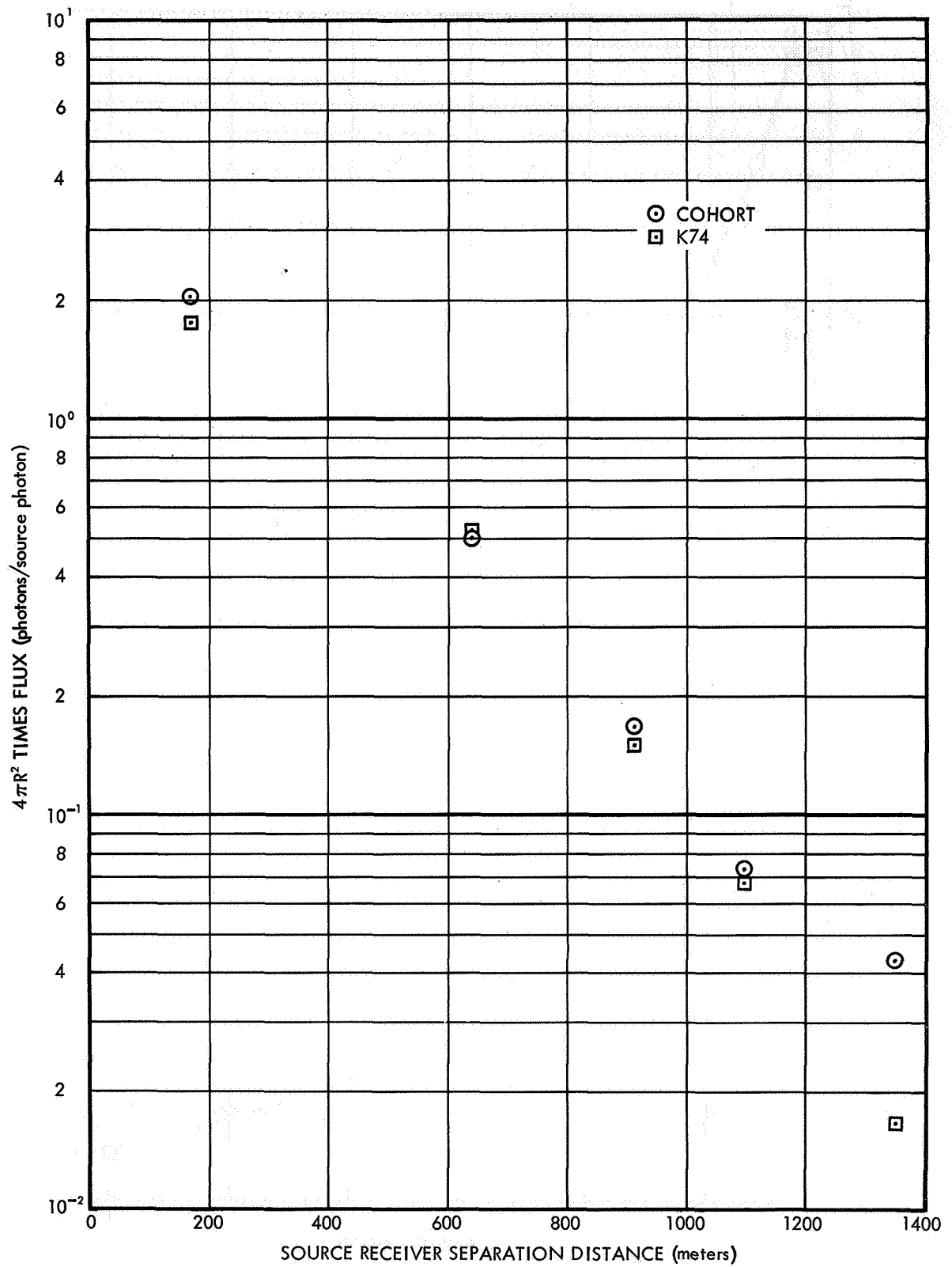


Fig. 11. $4\pi R^2$ Times the Photon Flux vs Distance from a 2 MeV Point Isotropic Gamma-Ray Source in an Infinite Medium of Air

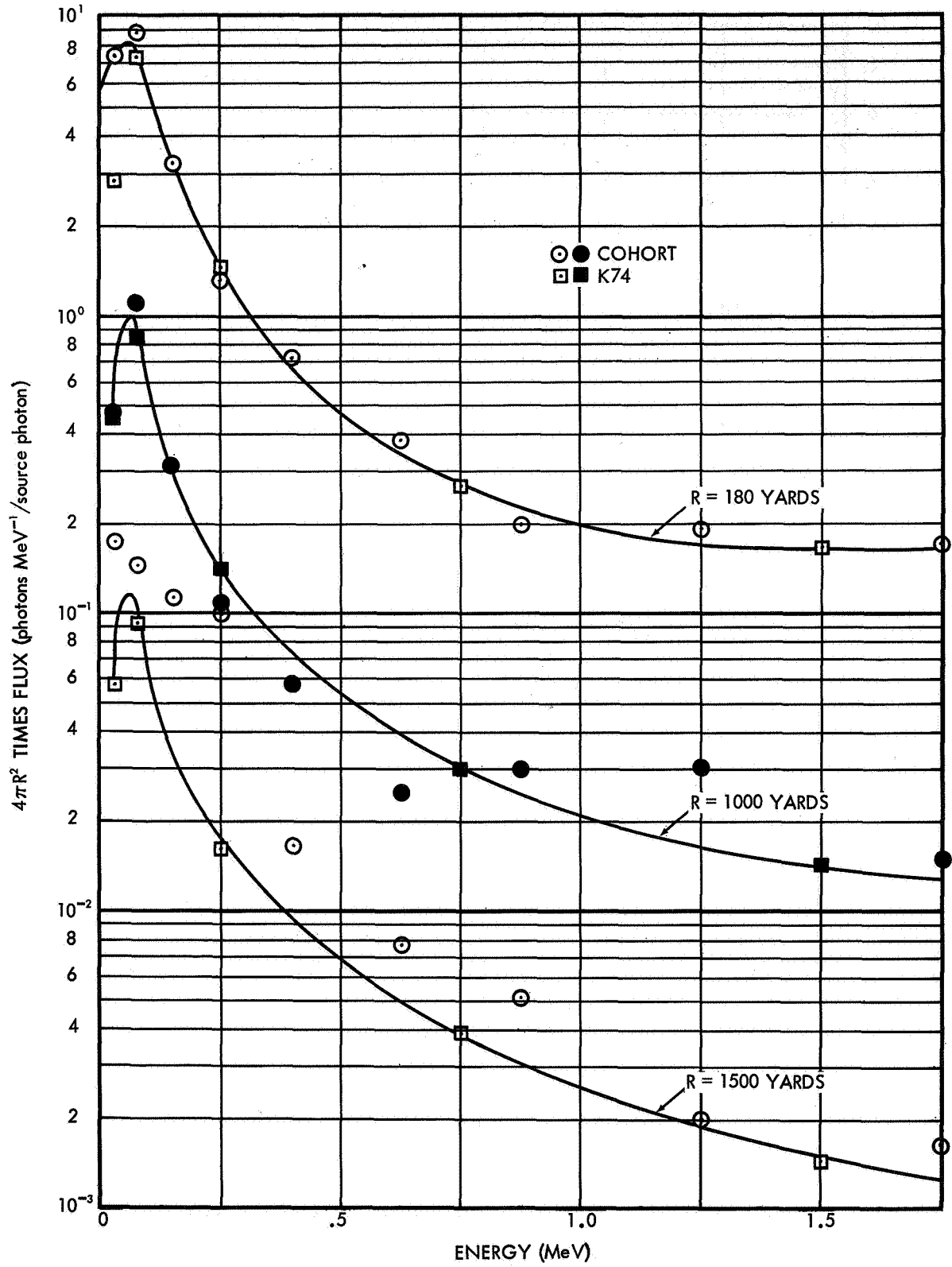


Fig. 12. $4\pi R^2$ Times Flux vs Energy at 180, 1000 and 1500 Yards from a 2 MeV Point Isotropic Gamma-Ray Source in an Infinite Medium of Air

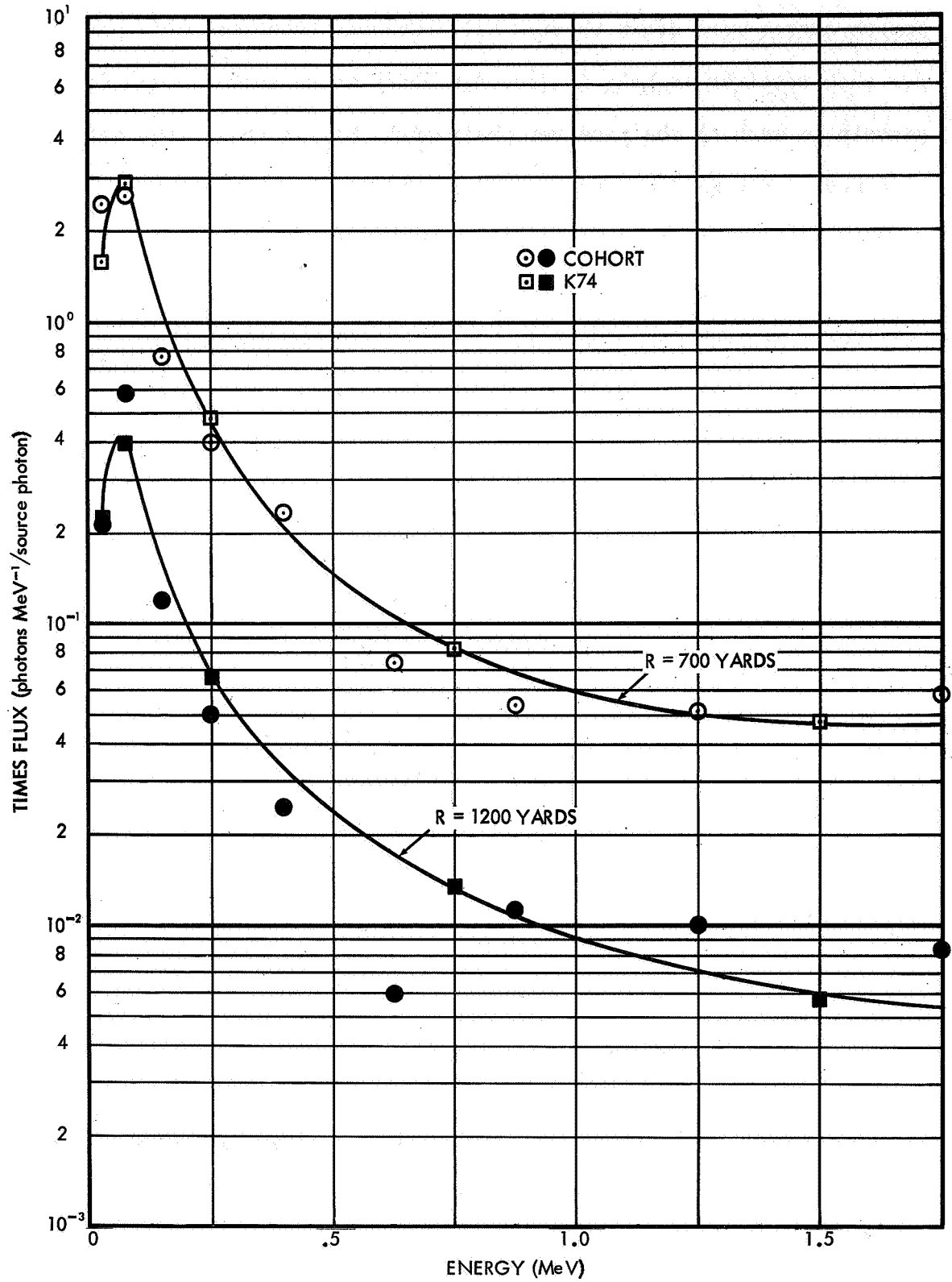


Fig. 13. $4\pi R^2$ Times Flux vs Energy at 700 and 1200 Yards from a 2 MeV Point Isotropic Gamma-Ray Source in an Infinite Medium of Air

Smooth curves were drawn through the combined COHORT and K-74 points for each receiver to help in distinguishing which sets of data points pertain to each of the receiver positions. More significance was attached to the K-74 points in drawing the smooth curves since the larger number of histories run with K-74 produced results with less statistical fluctuation. Note that for all but the largest source receiver distance, the COHORT points are fairly well distributed above and below the smooth curve indicating that the differences between the two sets of data are due to statistics.

3.8 Neutron Differential Number Spectra in Water

A problem was run with the H01 and A02 routines to calculate the differential number spectra at several distances from a 6-Mev point isotropic neutron source in an infinite medium of water. The COHORT data are compared with moments method data (Ref. 8) in Figures 14 through 18. The comparison is reasonably good for penetration distances of 10, 20 and 30 cm, but for 60 cm, the COHORT results are somewhat erratic. The erratic behavior of the COHORT data at a penetration distance of 60 cm is probably due to the small sample size (5040 histories) used and to the fact that no biasing was applied to obtain better statistics at penetration distances out to 60 cm. In the COHORT calculation the source particles were all started along the Z axis and the track lengths in spherical shell regions were recorded to give the differential number spectra at the different receiver positions.

A comparison of the spatial distribution of the fast-neutron dose rate as computed by both moments method and COHORT is presented in Figure 18. It is seen that the COHORT calculation underpredicts the moments

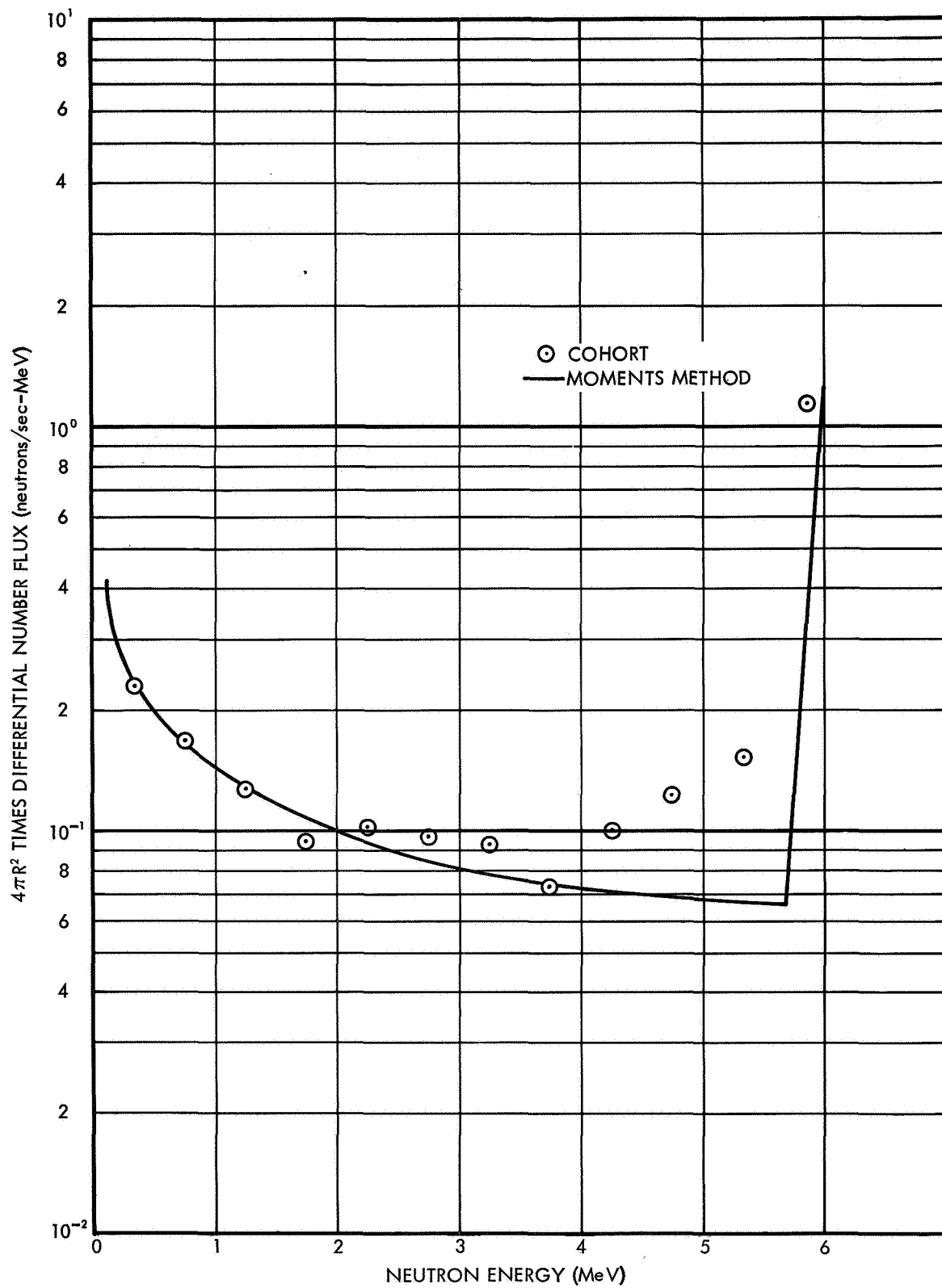


Fig. 14. Differential Number Spectra at 10 Cm: Point Isotropic 6 MeV Source in Water

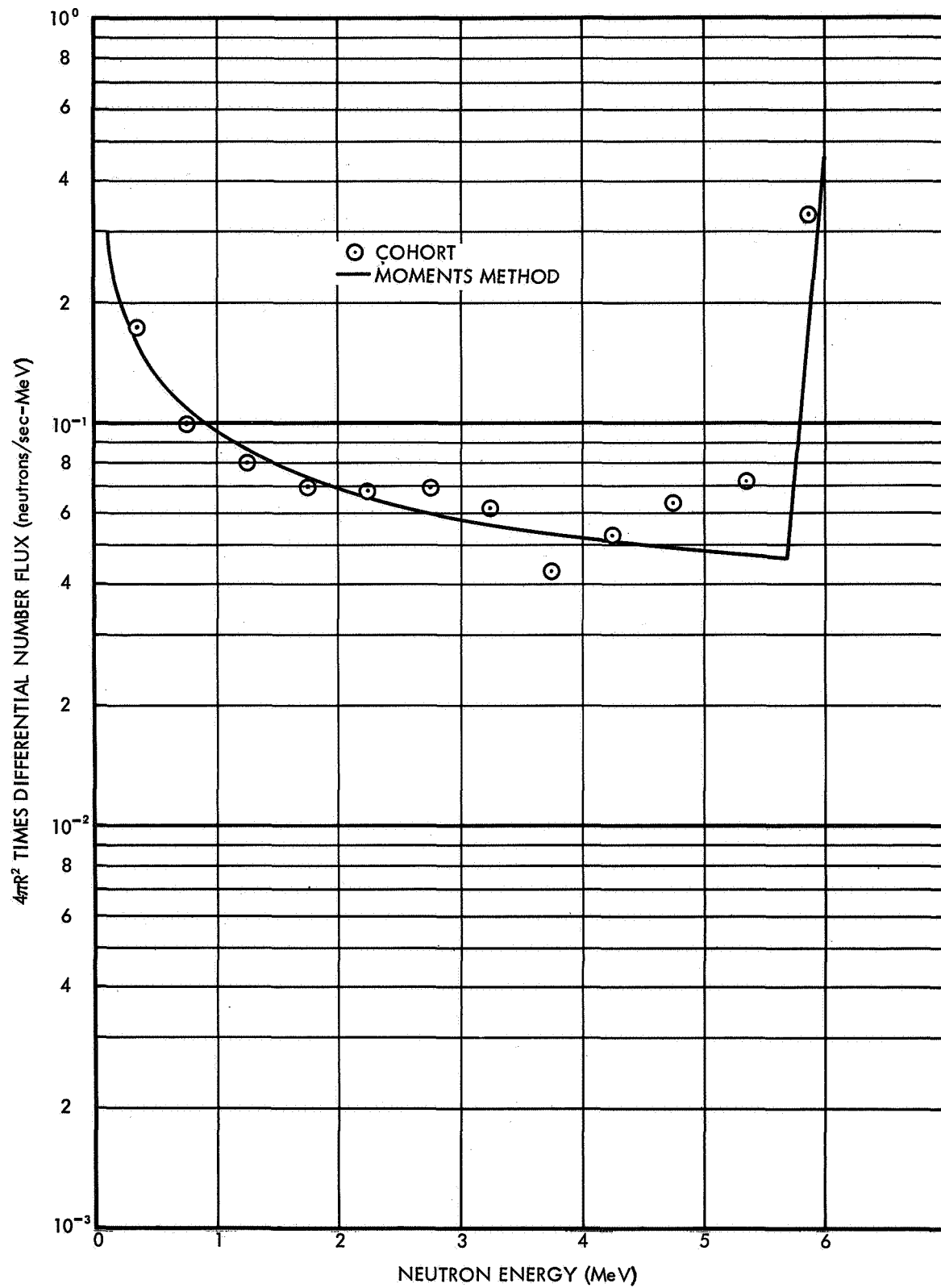


Fig. 15. Differential Number Spectra at 20 Cm: Point Isotropic 6 MeV Source in Water

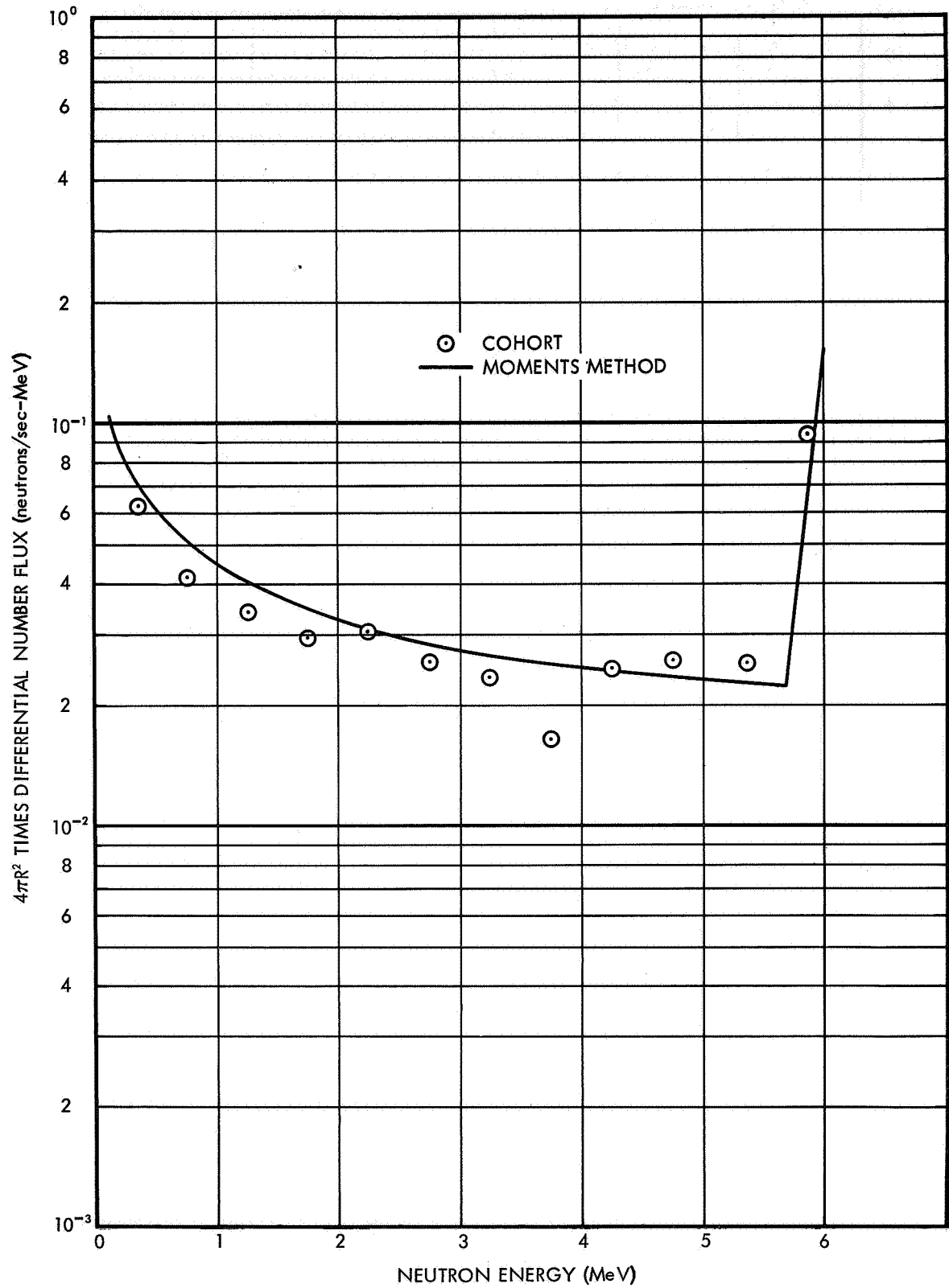


Fig. 16. Differential Number Spectra at 30 Cm: Point Isotropic 6 MeV Source in Water

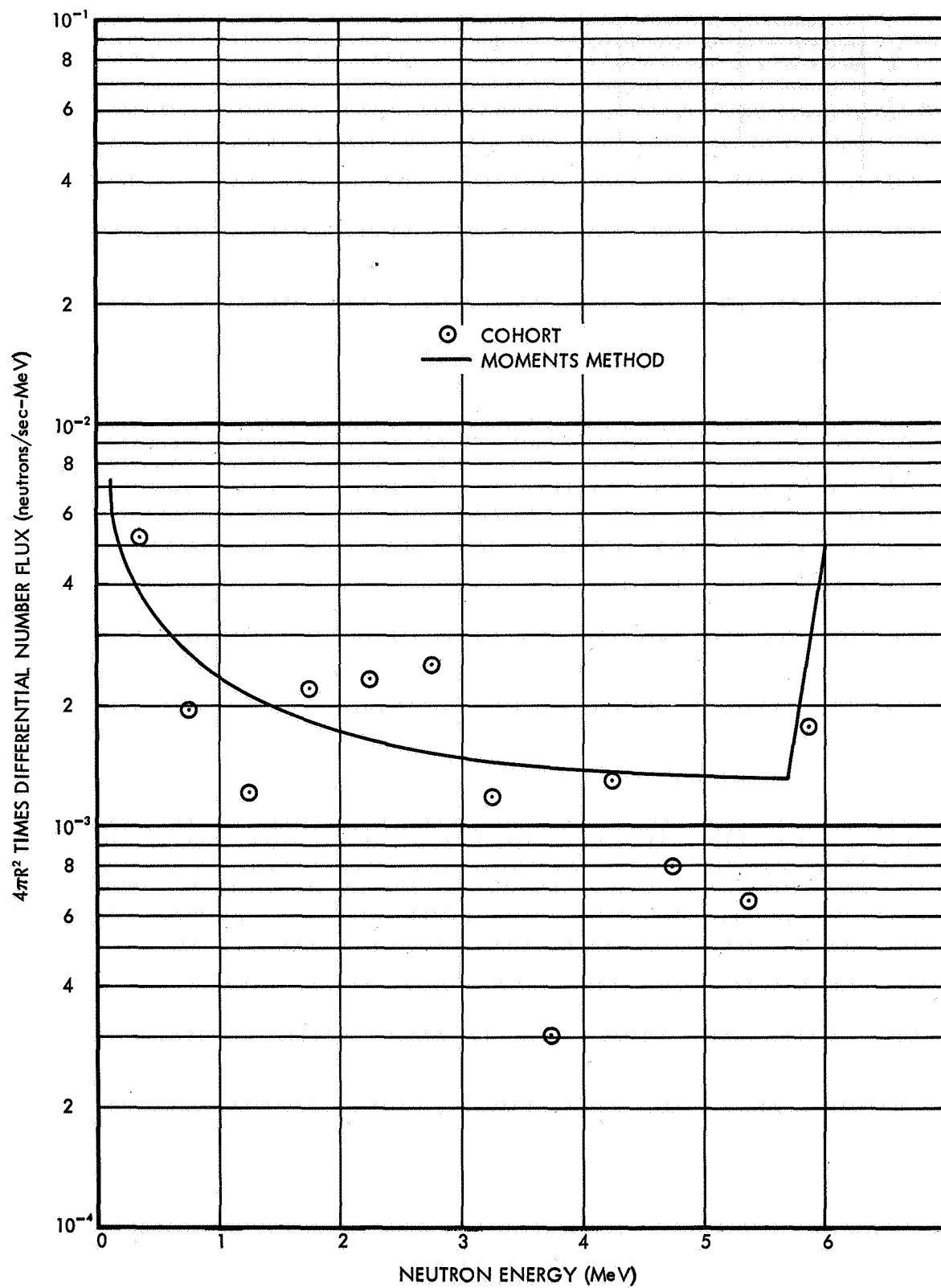


Fig. 17. Differential Number Spectra at 60 Cm: Point Isotropic 6 MeV Source in Water

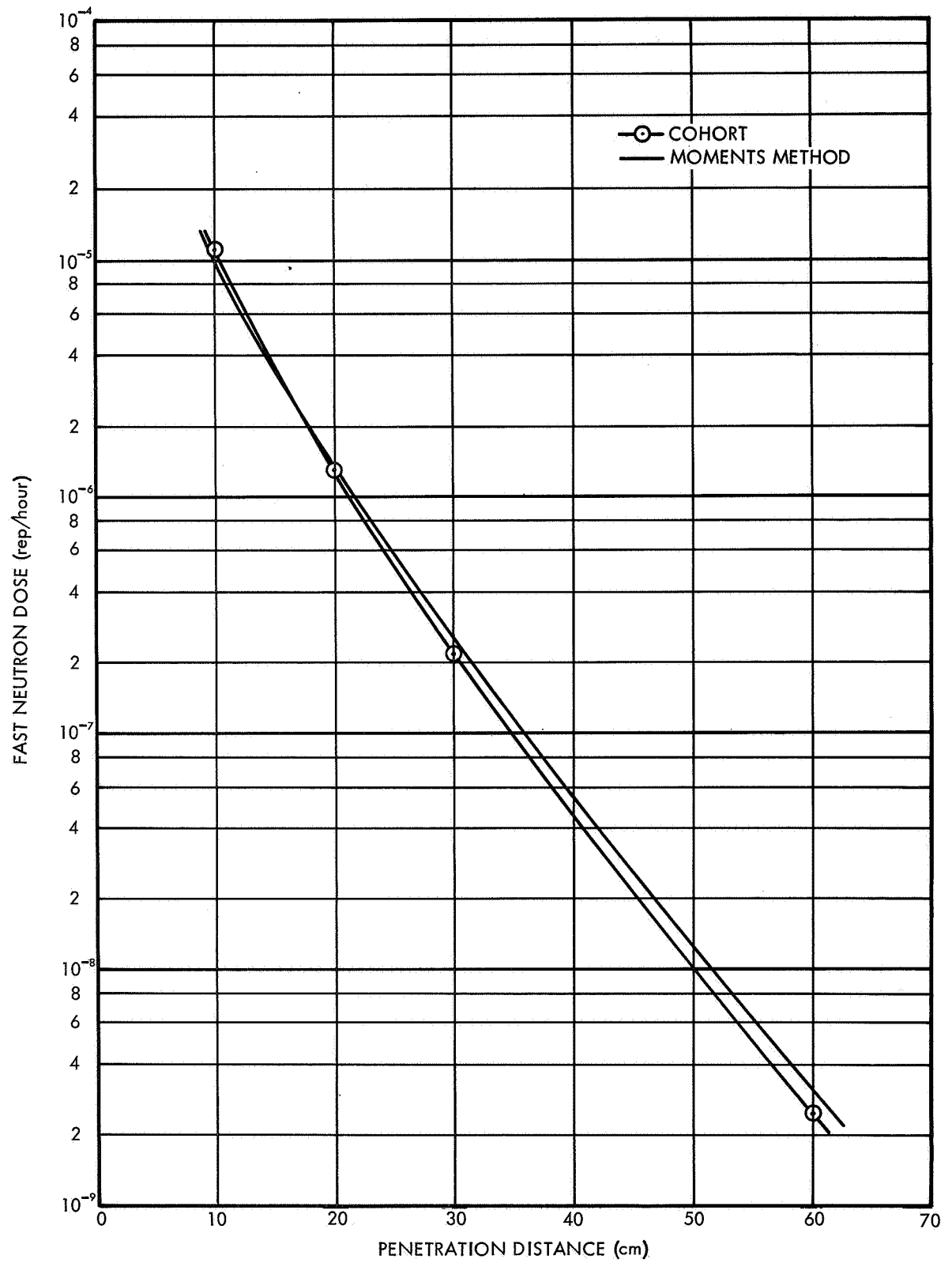


Fig. 18. Fast Neutron Dose in Water: 6 MeV Point Isotropic Source

method data by about 20% at penetration distances greater than 20 cm.

It is believed that the differences between the COHORT calculations and moments method data can be attributed mainly to differences in the cross sections used.

IV CONCLUSIONS AND RECOMMENDATIONS

The comparisons made between COHORT and other calculated data in Section III indicate that the COHORT program is capable of producing accurate results for a broad range of radiation transport problems. The COHORT program is versatile in that it will treat neutron and primary and secondary gamma radiation transport within complex geometries. The checkout problems shown in Section III are for the most part simple geometry problems. It is recommended that the COHORT program be tested using more complex geometric configurations.

In the process of checking out the COHORT program several possibilities of increasing the efficiency of the program were discovered but were not acted upon due to the limited amount of time and funds to perform the checkout. One such possibility is to modify the A01 and A02 analysis routines to preserve the 140 particle per batch structure that is employed in the H01 routine and to remove the necessity of sorting history tapes before using them in the analysis routines. This modification would do away with the need for the tape sort routine and would offer considerable time savings when running problems involving more than one energy super-group.

Another recommendation is that a set of library decks be prepared containing cross section information for those elements most commonly found in the materials used in reactors and reactor shielding. The availability of these library decks would greatly reduce the amount of time required to prepare the input data for the COHORT program.

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